AFRL-SR-AR-TR-10-0002

REPORT DOCUMENTATION PAGE

1. REPORT DATE (DD-MM-YYYY) 02-09-2009	**2. REPORT DATE** Final	**3. DATES COVERED:** *(From – To)* 01-06-05 - 31-08-09
4. TITLE AND SUBTITLE MULTISCALE MODELING OF METALLIC MICROSTRUCTURES: FROM DISLOCATIONS TO PLASTICITY		**5a. CONTRACT NUMBER**
		5b. GRANT NUMBER FA9550-05-1-0082
		5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S) Rickman, Jeffrey M. Haataja, Mikko P. Srolovitz, David J. Lesar, Richard A.		**5d. PROJECT NUMBER**
		5e. TASK NUMBER
		5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Lehigh University Bethlehem, PA 18015		**8. PERFORMING ORGANIZATION REPORT NUMBER**
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Office of Scientific Research 875 North Randolph Street Suite 325, Rm 3112 Arlington, VA 22203		**10. SPONSOR/MONITOR'S ACRONYM(S)** AFOSR
		AGENCY REPORT NUMBER

12. DISTRIBUTION AVAILABILITY STATEMENT
Public

13. SUPPLEMENTARY NOTES

20100204226

14. ABSTRACT

The goal of this research program has been to establish a quantitative link between important strengthening mechanisms and the observed stress-strain behavior of complex, metallic aerospace materials via a modeling strategy involving mesoscale dislocation dynamics (DD) simulations and spatial homogenization. In addition, we have sought to understand better the role of cracks and grain boundaries in determining mechanical behavior, and the impact of obstacles on the formation of dislocation substructures. Substantial progress has been made towards these ends by further developing the DD methodology, by elucidating the interactions among dislocations, solute, and extended defects, and by characterizing dislocation patterning resulting from interactions with obstacles. We summarize below the main results obtained under the auspices of this grant.

15. SUBJECT TERMS
mechanical properties, computer simulation

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
a. REPORT U	**b. ABSTRACT** U	**C. THIS PAGE** U	UU	5	Jeffrey M. Rickman
					20b. TELEPHONE NUMBER (Include area code) 610-758-4236

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI-Std Z39-18

Final Report
Multiscale Modeling of Metallic Microstructures: From Dislocations to Plasticity

AFOSR, FA9550-05-1-0082

J. M. Rickman

Department of Materials Science and Engineering and Department of Physics
Lehigh University
Bethlehem, PA 18015

M. Haataja

Dept. of Mechanical and Aerospace Engineering
Princeton University
Princeton, NJ 08544-5263

D. J. Srolovitz

Institute of High Performance Computing
1 Fusionopolis Way
#16-16 Connexis
Singapore 138632

R. LeSar

Dept. of Materials Science and Engineering
Iowa State University
Ames, IA 50011-2300

Objectives

The goal of this research program has been to establish a quantitative link between important strengthening mechanisms and the observed stress-strain behavior of complex, metallic aerospace materials via a modeling strategy involving mesoscale dislocation dynamics (DD) simulations and spatial homogenization. In addition, we have sought to understand better the role of cracks and grain boundaries in determining mechanical behavior, and the impact of obstacles on the formation of dislocation substructures. Substantial progress has been made towards these ends by further developing the DD methodology, by elucidating the interactions among dislocations, solute, and extended defects, and by characterizing dislocation patterning resulting from interactions with obstacles. We summarize below the main results obtained under the auspices of this grant.

Final Status of the Effort

Dislocation Dynamics Simulation – Level-Set Approach

We developed a parallel version of our level-set code and used this capability to study dislocation/obstacle interactions in which a deformable line passes through a sea of obstacles. In this work, the dislocation conformation changes in response to the elastic field of the obstacles, and both climb and glide motion are incorporated. With this code we have been able to move beyond older line-tension models of dislocation motion and therefore model more realistically hindered dislocation motion and associated strengthening behavior. In particular, it was found, somewhat counter-intuitively, that climb can reduce the effective glide mobility as dislocation lines find low-energy configurations when moving perpendicular to the glide plane.

In the future, we hope to build on this work to incorporate both non-random and mobile obstacle distributions. It is expected that these additions will result in more realistic models of dislocation/obstacle interactions that will permit the description of, for example, dynamic pinning/unpinning behavior associated with the Portevin-LeChatelier effect. Furthermore, the modeling of various spatial distributions of obstacles will allow us to identify those obstacle arrangements that lead to optimal pinning characteristics.

Crack/Solute Interactions

We have also developed a better understanding of the role of crack/solute interactions in determining material properties. The segregation of impurities to cracks influences crack stability and thereby the fracture toughness of a material. One important driving force for segregation is the long-ranged elastic interaction that results from misfitting solute atoms in the stress field of the crack. Thus, we have used simulation to examine these interactions.

In particular, to describe segregation in systems with stable cracks, we developed a novel, kinetic lattice-gas Monte Carlo simulation to describe quantitatively solute transport near a crack. In this model the crack is parameterized by a distribution of dislocations whose Burgers vectors adjust in response to loads (from solute and externally applied stresses) so as to maintain zero-traction boundary conditions. In a regime where crack loading is dominated by external tensile stresses, rate equations have been developed to describe the resulting biased diffusive flux. In a regime where solute loading becomes important, it is found that this loading enhances segregation and leads to small correlations in diffusive motion. In an extension of this work, we also examined diffusion in a system containing low-angle grain boundaries, as modeled by dislocation arrays.

Dislocation Patterning and Stress Correlations

We also examined the impact of obstacles, such as impurities and grain boundaries, on the formation of patterns in a system of mutually interaction dislocations. This was accomplished by characterizing the order in a pattern in terms of dislocation structure factors that reflect the tendency to form dislocation wall segments. We found that random stationary impurities frustrate wall formation without altering the characteristic length scale of the dislocation patterning, while grain boundaries promote dislocation wall formation via dislocation incorporation. By relating correlations in the dislocation density to stress correlations and invoking results from earlier studies of the random-field Ising model, we were also able to make some predictions for induced solute patterning in phase-separating alloys.

Unified Framework for Defect Energetics

We developed a unified framework for dislocation-based defect energetics, and validated our formalism by considering both the self- and interaction energies for combinations of cracks and grain boundaries. These extended defects were modeled as dislocation arrays, and this approach permits rapid calculation of defect energies. For example, grain-boundary energies as well as boundary interaction energies and crack/boundary energies, can be calculated with this formalism.

Accomplishments

In summary, our accomplishments during the period of this grant, include:

- the parallelization of our DD code and its application to investigate dislocation/obstacle interactions.
- the use of a lattice-gas Monte Carlo approach to study solute/crack interactions.
- the use of energy minimization to examine dislocation pattern formation in the presence of obstacles (including grain boundaries).
- the establishment of criteria for induced solute patterning in alloys.

- the development of a unified framework to calculate the self- and interaction energies of extended defects.
- the writing of a review of coarse-graining methodologies to link DD simulation with continuum descriptions of dislocation behavior.

Personnel

The following individuals are or have been involved in this effort.

Professor J. M. Rickman
Professor M. Haataja
Professor D. J. Srolovitz
Professor R. LeSar
Dr. Kevin T. Chu
Dr. Panya Kansuwan (Ph.D., Lehigh)
Mr. Zi Chen (graduate student, Princeton)

Publications

Several publications, resulting from the work performed under these auspices, are listed below.

"Unified Framework for Dislocation-Based Defect Energetics", J. M. Rickman, J. Vinals, and R. LeSar, Phil. Mag. **85**, 917-929 (2005).

"Issues in the Coarse Graining of Dislocation Energetics and Dynamics", J. M. Rickman and R. LeSar, Scripta Mater. **54**, 735-739 (2006).

"Biased Diffusive Transport and Solute Trapping Near a Crack", P. Kansuwan, J. M. Rickman, and T. J. Delph, Phys. Rev. B **75**, 024106 (2007).

"Impact of Obstacles on Dislocation Patterning and Stress Correlations", J. M. Rickman, M. Haataja, and R. LeSar, Phys. Rev. B **77**, 174105 (2008).

"Dislocation Pinning/Depinning by Impurities and Obstacles: A Level-Set Simulation Study," Z. Chen, K. T. Chu, M. Haataja, J. M. Rickman, and D. J. Srolovitz, submitted to Phys. Rev. B.

Interactions

Invited presentations include:

"Modeling of Dislocation Energetics and Dynamics" – Plasticity 2006, Halifax, NS (Summer 2006).

"Modeling of Dislocation Dynamics", SES meeting, Texas A&M, Fall 2007.

"Modeling of Dislocation Energetics and Dynamics" – Dept. of Physics, McGill University, Spring 2008.

"Local Stress and Elastic Constants", SIAM, Philadelphia, Spring, 2008.

"Modeling of Dislocation Energetics and Dynamics: Obstacles to Coarse Graining", SIAM, Philadelphia, Spring, 2008.

"3D Simulations of Evolving Dislocation Microstructures: Connection to Coarse Graining", MMM 2008, Tallahassee, FL, Fall 2008.

Inventions (none)

DTIC Final Technical Report
Profile Report

Date Published: 09/30/2009

Response 45699231

Page One

1. Principal InvestigatorName:

Jeffrey M. Rickman

2. Grant/Contract Title:

Multiscale Modeling of Metallic Microstructures: From Dislocations to Plasticity

3. Grant/Contract Number:

FA9550-05-1-0082

4. Reporting Period Start (MM/DD/YYYY):

01/06/2005

5. End (MM/DD/YYYY):

8/31/2009

6. Program Manager:

Dr. Joan Fuller

7. Distribution Statement (as on SF-298)

Distribution A - Approved for public release:

8. Annual Accomplishments (200 words maximum):

Our accomplishments over the course of this grant include:

- the parallelization of our DD code and its application to investigate dislocation/obstacle interactions.
- the use of a lattice-gas Monte Carlo approach to study solute/crack interactions.
- the use of energy minimization to examine dislocation pattern formation in the presence of obstacles (including grain boundaries).
- the establishment of criteria for induced solute patterning in alloys.
- the development of a unified framework to calculate the self- and interaction energies of extended defects.

- the writing of a review of coarse-graining methodologies to link DD simulation with continuum descriptions of dislocation behavior.

9. Archival Publications (published) during reporting period:

"Unified Framework for Dislocation-Based Defect Energetics", J. M. Rickman, J. Vinals, and R. LeSar, Phil. Mag. 85, 917-929 (2005).

"Issues in the Coarse Graining of Dislocation Energetics and Dynamics", J. M. Rickman and R. LeSar, Scripta Mater. 54, 735-739 (2006).

"Biased Diffusive Transport and Solute Trapping Near a Crack", P. Kansuwan, J. M. Rickman, and T. J. Delph, Phys. Rev. B 75, 024106 (2007).

"Impact of Obstacles on Dislocation Patterning and Stress Correlations", J. M. Rickman, M. Haataja, and R. LeSar, Phys. Rev. B 77, 174105 (2008).

"Dislocation Pinning/Depinning by Impurities and Obstacles: A Level-Set Simulation Study," Z. Chen, K. T. Chu, M. Haataja, J. M. Rickman, and D. J. Srolovitz, submitted to Phys. Rev. B.

10. Changes in research objectives (if any):

11. Change in AFOSR program manager, if any:

Dr. Joan Fuller is the current program manager.

12. Extensions granted or milestones slipped, if any:

An extension was granted in the fall of 2008.

13. Attach Final Report (max. 2MB)(If the report is larger than 2MB, please email file to program manager.)

(option:) file_42510_45699231_0_lafosr_2009.pdf

14. Please attach saved SF298 Form here:

(Please be sure to have already saved the SF298 Form, that you plan to attach to this survey, to your desktopso that it may be uploaded within this field.)

(option:) file_42510_45699231_1_sf298-2.doc